



ELSEVIER

Contents lists available at ScienceDirect

Physica E

journal homepage: [www.elsevier.com/locate/phys](http://www.elsevier.com/locate/phys)

# Armchair graphene nanoribbons under shear strain



Li-Hua Qu<sup>a</sup>, Jian-Min Zhang<sup>a,\*</sup>, Ke-Wei Xu<sup>b</sup>, Vincent Ji<sup>c</sup>

<sup>a</sup> College of Physics and Information Technology, Shaanxi Normal University, Xian 710062, Shaanxi, PR China

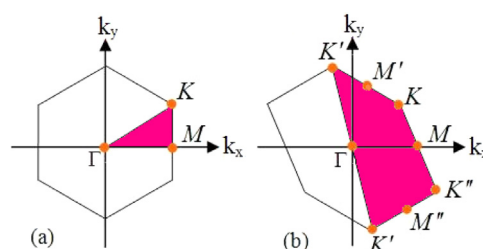
<sup>b</sup> College of Physics and Mechanical and Electronic Engineering, Xian University of Arts and Science, Xian 710065, PR China

<sup>c</sup> ICMMO/LEMHE, Université Paris-Sud 11, 91405 Orsay Cedex, France

## HIGHLIGHTS

- The symmetry of the hexagonal lattice is 2/m under shear strain.
- The stability improves with increasing ribbon width under the same shear strain.
- Shear strain makes the band structure a little smoother.
- The modification of the energy gap under shear strain is slight.

## GRAPHICAL ABSTRACT



The undeformed Brillouin zone (BZ) with 6/mmm hexagonal symmetry (panel (a)) and BZ deformed by shear strain with 2/m monoclinic symmetry (panel (b)).

## ARTICLE INFO

### Article history:

Received 16 December 2013

Received in revised form

20 February 2014

Accepted 24 February 2014

Available online 3 March 2014

### Keywords:

Armchair graphene nanoribbon

Shear strain

First-principle

## ABSTRACT

The symmetry and electronic properties of armchair graphene nanoribbons (AGNRs) have been investigated using density functional theory calculations. For the shear strained AGNRs, the D6h (6/mmm) symmetry of the hexagonal lattice further turns into 2/m. The stability improves with increasing ribbon width under the same shear strain. Besides, the modification of the energy gap under shear strain is weak.

© 2014 Elsevier B.V. All rights reserved.

## 1. Introduction

Graphene is a counterpart of graphite with well separated 2-D aromatic sheets composed of  $sp^2$ -bonded carbon atoms. Successful fabrication of graphene monolayers by means of mechanical exfoliation of graphite [1] or epitaxial growth on silicon carbide [2] has ignited tremendous interest in this material [3]. Its favorable characteristics such as chemical inertness, low dimensionality, extremely high mobility, and easy control of carriers by applied gate voltages, along with patterning using nanolithography, open

possibilities for further miniaturization of devices and the emergence of a carbon-based “post-silicon” electronics [2,4]. However, due to its gapless property, the modification of graphene is often needed for it to possess the different properties required for various potential applications, such as magnetic ordering for spintronics [5–10] and electron/spin transport properties including negative differential resistance [11–13]. Graphene nanoribbons (GNRs), which are slices of graphene, are a class of quasi one-dimensional (1D) structures with narrow widths and smooth edges, and are very promising materials for room temperature transistors with high switching speeds and carrier mobilities [14–16]. The unique properties of the GNRs are associated with their edge states; engineering the edge will affect its electronic properties. armchair GNRs (AGNRs), strips of graphene with widths on

\* Corresponding author. Tel.: +86 2985308456.

E-mail address: [jianm\\_zhang@yahoo.com](mailto:jianm_zhang@yahoo.com) (J.-M. Zhang).

the nanoscale, are one of the most widely investigated structures. By etching and patterning of graphene, GNRs can be feasibly fabricated. And armchair-edged gaps are dependent on the ribbon widths [17]; an observed experiment [18] has proved the previous theoretical prediction [17] that the energy gap decreases with increase of the graphene ribbons' width. The interesting band gap behavior gives rise to their potential application in AGNR based optoelectronic devices.

Many theoretical studies indicate that the strain effect is an effective way to modulate the electronic structures of nano-sheet and nanoribbon [19–21], and the band gap behavior of nanoribbon largely depends on both their edge structures and widths [17,20–25]. For example, in the elastic deformation range, the energy band gap of zigzag GNRs is less sensitive to the uniaxial strain, while the band gap of armchair GNRs exhibits a sawtooth-shaped oscillation [20], blocking their applications. The shear modulus of graphene has been reported using various approaches. By using the molecular mechanics method, Sakhaee-Pour [26] reported the shear modulus of zigzag and armchair structures to be 0.213 and 0.228 TPa, respectively. Even though the shear modulus of graphene has been reported using several approaches, the strength and fracture strain of graphene under shear have not been reported so far.

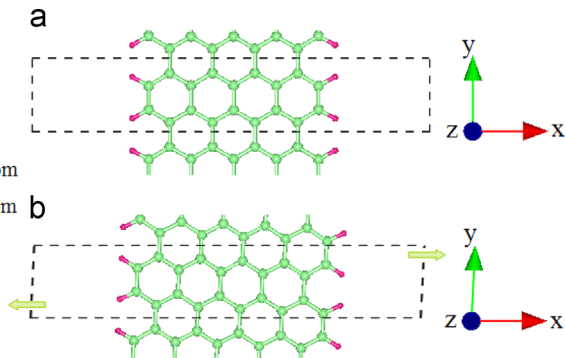
In this work, we focus on the AGNR. We have numerically investigated the symmetry, stability and electronic properties of AGNRs under shear strain using a first-principle method. The rest of the paper is organized as follows. In Section 2, the calculation methods of AGNRs are described in detail. In Section 3, the symmetry, stability and electronic properties of AGNRs under shear strain are analyzed and discussed. Finally, the conclusions of the work are presented in Section 4.

## 2. Methods

Here, we will take the optimized geometrical structures of 9-AGNR terminated with H atoms as examples. This bandwidth is large enough to prevent interactions between C and H atoms on both edges, so the geometrical structures of 9-AGNR under shear strains can represent other structures (12-AGNR, 15-AGNR, etc.). The unstrained and the shear strain of 5% systems are shown in Fig.1(a) and (b) respectively. For the central scattering region, the presence of a shear strain changes the coordinates of the  $i$ th atom according to following relation:

$$x_i = x_i^{(0)} + \gamma y_i^{(0)} \quad (1)$$

where  $\gamma$  is the applied shear strain. The superscript (0) denotes the unstrained states. The  $y$ -component of the atom coordinates is free



**Fig. 1.** Schematic views of 9-AGNR. (a) The unstrained 9-AGNR. (b) 9-AGNR under a shear strain of  $\gamma=5\%$ . The edge carbon atoms (green circles) are passivated by hydrogen atoms (pink circles). The insides of parallelograms denote the unit cells of the systems. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

to relax. The examples are illustrated in Fig. 1 to show the deformation.

All calculations have been performed using the density functional theory [27,28] as implemented in the Vienna ab initio simulation package (VASP) [27–31]. The Perdew–Burke–Ernzerhof (PBE) theory of the generalized gradient approximation (GGA-PBE) has been used for the exchange and correlation functional within the projector-augmented wave (PAW) [32] framework. A vacuum thickness of 20 Å in the  $z$ -direction normal to the surface is used to decouple the periodic images. A  $1 \times 40 \times 1$  Monkhorst–Pack  $k$ -mesh [33] is used to sample the Brillouin zone with cutoff energies of 450 eV. During relaxations, the positions of all atoms are allowed to fully relax until the force on each atom is less than 0.01 eV between two ionic steps and the convergence of the electronic self-consistent energy is less than  $10^{-5}$  eV.

## 3. Results and discussions

### 3.1. The symmetry and stability

The in-plane elastic behavior of the honeycomb lattice is isotropic. According to the Cauchy–Born rule, when straining a graphene sample its lattice vectors are affected accordingly, as well as the associated reciprocal vectors. This can be explained by tight-binding (TB) approximation with the following introduction:

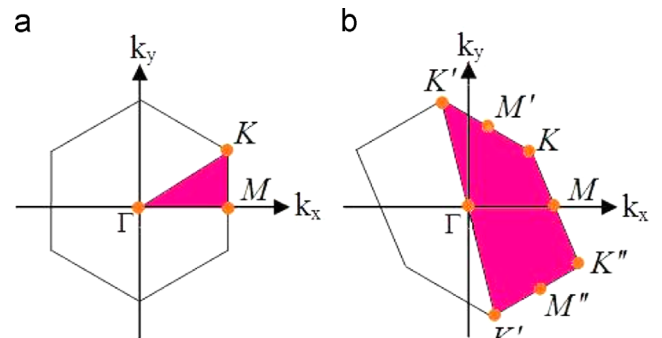
$$kr = k(I + \epsilon)r_0 = [(I + \epsilon)^T k]r_0 = k^*r_0 \quad (2)$$

where  $k$  and  $k^*$  can be regarded as the reciprocal vector in the deformed space and the undeformed reciprocal vector, respectively,  $I$  is the unit matrix,  $\epsilon$  is the strain tensor, and  $r$  and  $r_0$  are real space vectors. Subscript “0” denotes undeformed states. The introduction of  $k^*$  and the property in Eq. (2) greatly facilitate the analysis. For example, the TB Hamiltonian becomes

$$H(k) = \sum_{i=1,2,3} t_i \exp(ika_i) = \sum_{i=1,2,3} t_i \exp(k^*a_{i0}) \quad (3)$$

where  $a_i$  are three bond vectors from a carbon atom, and  $t_i$  are hopping parameters which depend on the bond length. This incorporates the effect of strain into the variation of  $t_i$ . When a symmetric strain is applied,  $t_1 = t_2 = t_3$ , and the Fermi points (synonymous with the Dirac points in this paper)  $k_F$ , defined by  $E(k_F) = |H(k_F)| = 0$ , sit at the vertex of the hexagonal Brillouin zone (BZ), i.e., the  $K$  points in Fig. 2(a). For shear strains which are asymmetric,  $t_1$ ,  $t_2$  and  $t_3$  are no longer equal, and the Fermi points will deviate from  $K$  in the  $k^*$  space.

By applying the shear strain given in Eq. (1) to the graphene lattice, the 6/mmm symmetry of the hexagonal lattice (Fig. 2(a)) is further lowered to monoclinic. The corresponding symmetry



**Fig. 2.** Brillouin zone of graphene. The shaded areas are the corresponding irreducible part: (a) undeformed BZ with 6/mmm hexagonal symmetry and (b) BZ deformed by shear strain with 2/m monoclinic symmetry.

Download English Version:

<https://daneshyari.com/en/article/1544248>

Download Persian Version:

<https://daneshyari.com/article/1544248>

[Daneshyari.com](https://daneshyari.com)